

Reply to a Comment of M. Continentino on “Universally diverging Grüneisen parameter and the magnetocaloric effect close to quantum critical points”

Lijun Zhu¹, Markus Garst², Achim Rosch³, and Qimiao Si¹

¹Department of Physics & Astronomy, Rice University, Houston, TX 77005-1892, USA

²Institut für Theorie der Kondensierten Materie,
Universität Karlsruhe, D-76128 Karlsruhe, Germany

³Institut für Theoretische Physik, University of Cologne, 50937 Köln, Germany

We show that the comment [cond-mat/0408217] by Continentino on our recent paper [PRL **91**, 066404 (2003)] reaches incorrect conclusions as the comment wrongly extrapolates from results valid close to a classical phase transition into the quantum critical regime.

In his comment [1] and a previous preprint [3] Continentino claims that our result [2] for the quantum-critical Grüneisen ratio $\Gamma = \frac{\alpha}{c_p} \sim T^{-1/(\nu z)}$ (where α and c_p are thermal expansion and specific heat, respectively) should be replaced by $\Gamma \sim T^{-1/\psi}$, where ψ is the shift exponent. We explain below why this claim is incorrect above the upper critical dimension, *i.e.* $d + z > 4$. Below the upper critical dimension, one has $\psi = \nu z$ and no discrepancy arises.

We will focus on the *quantum critical regime*, about which the comment raises the issue; the experiments reported in Ref. [4] also concern this regime. Above the upper critical dimension ($d + z > 4$), a scaling analysis (see below) is more subtle due to the presence of some dangerously irrelevant variable(s), but a direct calculation of Γ in the quantum critical regime is straightforward. Therefore we reported in [2] the results of explicit calculations for spin-density-wave (SDW) quantum critical points (QCPs) [6, 7, 8], where the quartic coupling is dangerously irrelevant and $\psi \neq \nu z$. For instance, for $d = 3$ and $z = 2$ where the exponents $\psi = 2/3$ and $\nu z = 1$, we find $\Gamma \sim T^{-1}$ while Continentino would predict $\Gamma \sim T^{-3/2}$. These calculations already show that the claim of Continentino is incorrect.

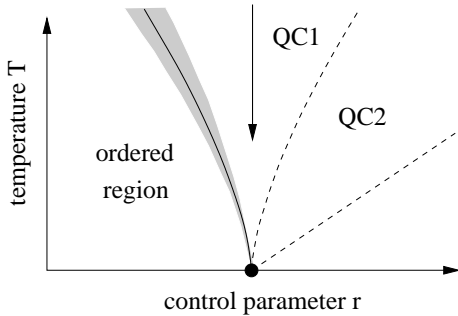


FIG. 1: Schematic phase diagram near a quantum-critical point. In the shaded area, classical scaling is expected. The temperature dependence in the quantum critical regime is measured along a path indicated by the arrow. The dashed lines, defined for positive r , describe the upper and lower crossover temperatures, $T_{cr1} \propto (r/u)^\psi$ and $T_{cr2} \propto r^{\nu z}$, respectively.

It is straightforward to pin down why the rather general argument given in the comment fails. The reason is that both the Ehrenfest relation [1] and the scaling ansatz used in Ref. [3] [Eq. (5) of Ref. [3]; the ansatz is a special form of Eq. (1.30) in Ref. [5]] are only valid close to the *classical* phase transition, *i.e.* in the shaded area shown in Fig. 1, but not in the quantum critical region. The part of the calculation of Ref. [2] under discussion is, however, performed along the arrow depicted in Fig. 1 which never enters the shaded region.

The problem with Continentino’s approach can be traced back to the qualitatively different role which the quartic coupling $u > 0$ of magnetic fluctuations plays in the classical critical and quantum critical regimes: it is a relevant coupling in the former but (dangerously) irrelevant in the latter. This makes it incorrect to use the simple scaling form Eq. (5) of Ref. [3] to describe all the regimes. Instead, one has to include explicitly the quartic coupling u in the scaling ansatz for the free energy

$$F \approx T^{\frac{d+z}{z}} f\left(\frac{r}{T^{1/(\nu z)}}, uT^{\frac{d+z-d}{z}}\right) \quad (1)$$

where $r \propto p - p_c$ measures the distance from the QCP. We assume $d + z > 4$, $d > 1/\nu$ and $d \neq z$ to avoid logarithmic terms. In the quantum critical regimes QC1 and QC2, $|x|, y \ll 1$ and $x + y \gg y^{\frac{1}{\nu(4-d)}}$, one obtains (omitting all multiplying constant factors) $f(x, y) \approx 1 + x + y$. (x and y appear separately in the Fermi liquid regime below QC2.) In contrast, the scaling ansatz [3, 5] of Continentino $f \propto |x + y|^{2-\tilde{\alpha}}$, can only be valid within the Ginzburg region of the classical transition (shaded area in Fig. 1), *i.e.* only for $|x + y| \ll y^{\frac{1}{\nu(4-d)}}$ for $d < 4$ (see, *e.g.*, Ref. [7]). The use of this formula outside of its range of applicability in region QC1 (as done in Refs. [3, 5] and implicitly when comparing our results to the Ehrenfest relation in Ref. [1]) implies that $F \propto u^{2-\tilde{\alpha}} T^{\frac{\tilde{\alpha}-\alpha}{\nu z} + \frac{2-\tilde{\alpha}}{\psi}}$ for $r = 0$. This result is wrong on two accounts. First, it entirely misses the leading term which corresponds to Gaussian critical fluctuations [cf. the “1” term in the expression for $f(x, y)$ above]. Second, it is incorrect even for the sub-leading term for $\psi \neq \nu z$ as it depends explicitly on the exponent $\tilde{\alpha}$ which characterizes only the *classical* but not the quantum-critical transition

(in some cases, e.g. for $d = 2$ and Heisenberg symmetry, a classical transition does not even exist). It therefore also contradicts numerous results in the literature, e.g. Refs. [7, 8].

In his comment [1] Continentino stated that Gaussian fluctuations should not be taken into account in the scaling analysis. This is incorrect, since Gaussian fluctuations are part of the singular contributions at the QCP and in fact the leading singular terms in the QC1 and QC2 regions. As explained above, the dominance of the Gaussian fluctuations in QC1 and QC2 is fully compatible (see e.g. Refs. [7, 8]) with both the existence of a Néel line and $\psi \neq \nu z$ due to the dangerously irrelevant variable u .

To summarize, the comment [1] reaches incorrect conclusions by extrapolating from results valid very close to the classical phase transition into the quantum critical regime where they are not valid. Furthermore the

scaling ansatz used in Refs. [3, 5] incorrectly treats the dangerously irrelevant quartic coupling above the upper critical dimension.

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